Impurity spin dynamics in 2D antiferromagnets and superconductors

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We discuss the universal theory of localized impurities in the paramagnetic state of 2D antiferromagnets where the spin gap is assumed to be significantly smaller than a typical exchange energy. We study the impurity spin susceptibility near the host quantum transition from a gapped paramagnet to a Néel state, and we compute the impurity-induced damping of the spin-1 mode of the gapped antiferromagnet. Under suitable conditions our results apply also to d-wave superconductors.

Doped antiferromagnets (AF) have been the subject of intense studies in the context of the cuprate high-temperature superconductors and other layered transition metal compounds. We present a quantum theory of a particular class of doped AF where it is possible to neglect the coupling between the spin and charge degrees of freedom and consider a theory of the spin excitations alone. Such a theory will apply to (i) quasi-2D 'spin gap' insulators like $SrCu_2O_3$ or NaV_2O_5 in which a small fraction of the magnetic ions (Cu or V) are replaced by non-magnetic ions like Zn or Li and to (ii) high-temperature superconductors like $YBa_2Cu_3O_7$ in which a small fraction of Cu has been replaced by non-magnetic Zn or Li. In the first case the spin gap Δ is significantly smaller than the charge gap justifying a theory of the spin excitations alone. In the second situation the effect of the fermionic quasiparticles in the superconducting state can be shown [1] to be weak due to the linearly vanishing density of states of the Fermi level.

The effect of a (magnetic or non-magnetic) impurity can be probed by measuring the uniform spin susceptibility, which takes the form $\chi = (g\mu_B)^2(A\chi_b + \chi_{\rm imp})$ where A is the total area of the AF, χ_b is the bulk response per unit area, and $\chi_{\rm imp}$ is the additional impurity contribution. In the paramagnetic ground state of the host each impurity induces a distortion of the host spin arrangement with a net magnetic moment S associated with the impurity. The distortion is *confined* to the vicinity of the impurity which implies that the impurity susceptibility follows

$$\chi_{\rm imp} = \frac{S(S+1)}{3k_BT} \quad \text{as} \ \ T \to 0. \tag{1}$$

For a non-magnetic impurity in a spin-1/2 system we have $S = 1/2$; for a general impurity eq. (1) can be used as definition of S.

The basis of our investigations is a boundary quantum field theory which describes a bulk AF together with arbitrary localized deformations. We focus on the vicinity of a quantum transition from a paramagnet to a magnetically ordered Néel state: Then the spin gap in the paramagnetic state is small compared to a typical nearest-neighbor exchange, $\Delta \ll J$, which is the situation realized in many compounds. The field theory has been discussed in Ref. [1]; it consists of $d+1$-dimensional ϕ^4 theory for the bulk ordering transition and a coupling to a local quantum impurity spin. The renormalization-group (RG) analysis shows that both the bulk and the boundary couplings are marginal for $d = 3$ and flow to fixed-point values for $d < 3$. This implies that the coupling between the bulk and impurity excitations becomes *universal*, and the spin dynamics in the vicinity of the impurity is completely determined by bulk parameters, the gap Δ and the velocity of spin excitations c. Based on the RG results one obtains a number of universal properties in an expansion in $\epsilon = 3 - d$; we mention here the behavior of the uniform susceptibility at the bulk critical point. The system shows the Curie response of an *irrational* spin as $T \to 0$,

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$\chi_{\rm imp} = \mathcal{C}_1/(k_B T)$, where $\mathcal{C}_1$ is a *universal* number independent of microscopic details. The ϵ expansion result for $\mathcal{C}_1$ is

$$\mathcal{C}_1 = \frac{S(S+1)}{3}\left[1 + \left(\frac{33\epsilon}{40}\right)^{1/2} - \frac{7\epsilon}{4} + ...\right]. \qquad (2)$$

More detailed dynamic information can be obtained by a self-consistent diagrammatic method. The paramagnetic phase of the bulk is assumed to be dimerized, its spin-1 excitations can be described using triplet bosons $t_{\mathbf{k}\alpha}$. The impurity is represented by an additional spin S_α at site 0,

$$H = \sum_{\mathbf{k},\alpha} \epsilon_{\mathbf{k}} t^\dagger_{\mathbf{k}\alpha} t_{\mathbf{k}\alpha} + \frac{K}{\sqrt{N_s}} \sum_{\mathbf{k}\alpha} S_\alpha \frac{t^\dagger_{\mathbf{k}\alpha} + t_{\mathbf{k}\alpha}}{\sqrt{\epsilon_{\mathbf{k}}/J}} \qquad (3)$$

where J is the host exchange constant, $\epsilon_{\mathbf{k}}$ the energy of the spin-1 mode in the bulk, K the coupling constant to the impurity spin, and N_s the number of lattice sites. The impurity spin is represented by auxiliary fermions f, the impurity dynamics is contained in the fermion self-energy which arises from the scattering off the t bosons. We employ a self-consistent non-crossing approximation (NCA) to calculate this self-energy; this approach follows from a saddle-point principle after generalizing the spin symmetry to SU(N) and taking the limit $N \to \infty$. The NCA equations can be solved in the scaling limit; the value of the coupling K drops out of all results for physical observables provided that $\Delta \ll J$ – we obtain the same universal behavior as predicted by the RG. In fact, the results for susceptibility and impurity spin correlations agree with the one-loop RG result [1].

The diagrammatic approach can be easily applied to a system with a finite density of impurities $n_{\rm imp}$. The important observation is that the impact of the impurities is determined by a single energy scale $\Gamma \equiv n_{\rm imp}(\hbar c)^d/\Delta^{d-1}$. The AF in the absence of impurities shows a pole in the dynamic susceptibility $\chi_{\mathbf{Q}}(\omega)$ at the AF wavevector $\mathbf{Q}$. Our main concern is the fate of this collective peak upon the introduction of impurities. Scaling arguments predict that the susceptibility takes the form

$$\chi_{\mathbf{Q}}(\omega) = \frac{\mathcal{A}}{\Delta^2}\Phi\left(\frac{\hbar\omega}{\Delta}, \frac{\Gamma}{\Delta}\right) \quad (T=0)\,, \qquad (4)$$

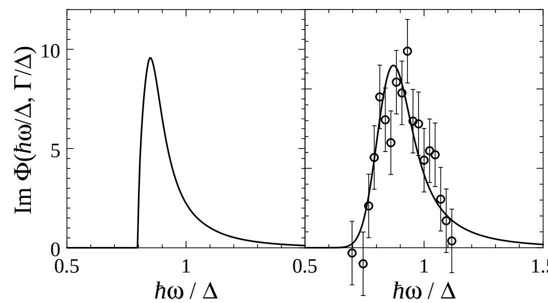

Figure 1. Left: Universal lineshape ImΦ for $\Gamma/\Delta = 0.125$. Right: The same, but convoluted with a Gaussian corresponding to the experimental resolution of [2], together with the data points of Ref. [2]. We have used $\Delta = 43$ meV – this small shift may be attributed to perturbations being irrelevant in the RG sense.

where Φ is a universal function, and $\mathcal{A}$ denotes the quasiparticle weight. In the absence of impurities we have $\Phi(\overline{\omega}, 0) = 1/(1-(\overline{\omega}+i0^+)^2)$. The self-energy of the spin-1 bosons caused by the scattering at randomly distributed impurities is calculated using a self-consistent Born approximation. The equations for the Green's functions can be entirely written in terms of scaling functions with arguments $\hbar\omega/\Delta$ and Γ/Δ, consistent with the scaling prediction (4). A numerical result for Φ is shown in Fig. 1. The quasiparticle pole is broadened to an asymmetric line, with a tail at high frequencies. Our theory can be applied to a recent experiment [2] where the inpurity-induced broadening of the spin-1 'resonance peak' at energy $\Delta = 40$ meV in $YBa_2Cu_3O_7$ has been observed. This experiment has $n_{\rm imp} = 0.005$, $\Gamma = 5$ meV, $\Gamma/\Delta = 0.125$. The half-width of the line is approximately Γ, and this is in excellent accord with the measured linewidth of 4.25 meV, see Fig. 1. More tests of the predictions of our theory should be possible in the future.

REFERENCES

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